Phase Diagram of $S = 1$ Bond-Alternating XXZ Chains Reflecting the Hidden $Z_2 \times Z_2$ Symmetry

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The phase diagram of the spin-1 bond-alternating XXZ chain is studied numerically. This model is appropriate to study the VBS picture and the hidden $Z_2 \times Z_2$ symmetry concerning to the Haldane gap problem. The possible phases are the ferromagnetic, the XY, the Haldane, the dimer, and the Néel ones. The critical properties of this model can be interpreted as the Ashkin-Teller type reflecting the hidden $Z_2 \times Z_2$ symmetry. The phase transitions are of the Berezinskii-Kosterlitz-Thouless type (XY-Haldane and XY-dimer), of the 2D Gaussian type (Haldane-dimer), and of the 2D Ising type (Haldane-Néel and dimer-Néel). We determine the phase boundary and universality class using the recent developed techniques by the authors.

KEYWORDS: Haldane gap, $S = 1$ bond-alternating XXZ chain, Hidden $Z_2 \times Z_2$ symmetry, BKT transition, Gaussian transition

§1. Introduction

Haldane[1)] made a fascinating conjecture that the integer spin S Heisenberg antiferromagnetic chain has a unique disordered ground state with an energy gap, while for a half odd integer S it is critical without energy gap and belongs to the same universality class as the $S = 1/2$ case. For $S = 1$, this conjecture is practically established by many numerical[2,3)] and experimental[4,5,6)] studies. Affleck *et. al.*[7)] proposed the valence bond solid (VBS) state for the Haldane gap systems. They studied a $S = 1$ isotropic spin chain with special biquadratic interactions and constructed the exact ground state whose spin correlation decay exponetially. They also showed the existance of a finite gap for the excitation.

For this problem, den Nijs and Rommelse[8)] proposed the string order parameter,

$$\mathcal{O}^{\alpha}_{\text{string}} = -\lim_{|j-k|\to\infty} \left\langle S^{\alpha}_{j} \exp\left[i\pi \sum_{l=j+1}^{k-1} S^{\alpha}_{l} \right] S^{\alpha}_{k} \right\rangle \quad (1.1)$$

(where $\alpha = z, x$ and $\langle\cdot\rangle$ means an expectation in the ground state) which measures the hidden antiferromagnetic order and characterizes the $S = 1$ Haldane phase. By the Goldstone's theorem, if some symmetry is broken in the Haldane gap system, it is not expected a continuous one. Later, the string order parameter was related to the hidden discrete $Z_2 \times Z_2$ symmetry by Kennedy and Tasaki[9)]. Using a nonlocal unitary transformation, they transformed the $S = 1$ spin chains to one model which has local interactions and the discrete symmetry explicitly. The string order parameters are transformed to the ferromagnetic ones, and they relate to the hidden $Z_2 \times Z_2$ symmetry.

In our previous paper[10)] with Okamoto, we have studied the $S = 1$ XXZ spin chain with bond alternation,

$$H = \sum_{j=1}^{N} (1 - \delta(-1)^j)[S^x_j S^x_{j+1} + S^y_j S^y_{j+1} + \Delta S^z_j S^z_{j+1}], \quad (1.2)$$

and found that the phase diagram reflects the hidden $Z_2 \times Z_2$ symmetry. The possible phases are the ferromagnetic, the XY, the Haldane, the dimer, and the Néel ones (Fig.1). For $\delta = 0$, many numerical studies have been done. The Haldane-Néel transition occurs at $\Delta_{c1} = 1.17 \pm 0.02$ and belongs to the 2D Ising universality class[11,12,13,14)]. Near $\Delta = \Delta_{c1}$, the energy gap behaves as $|\Delta - \Delta_{c1}|$, so the critical exponent ν is 1. At $\Delta = 0$ precisely, the Haldane-XY transition occurs and it is of the Berezinskii-Kosterlitz-Thouless (BKT) type[10)]. For this transition, the energy gap closes as $\exp(-\text{const}/\sqrt{\Delta})$, and in the XY phase the excitation is gapless. In the Haldane phase ($0 < \Delta < \Delta_{c1}$) the hidden $Z_2 \times Z_2$ symmetry is fully broken and the string order parameters $\mathcal{O}^{\alpha}_{\text{string}}$ ($\alpha = z, x$) have finite values, while in the Néel phase ($\Delta_{c1} < \Delta$) the discrete symmetry is partially broken and $\mathcal{O}^{z}_{\text{string}}$ is non zero but $\mathcal{O}^{x}_{\text{string}} = 0$[9)]. Introducing δ, we expect the dimer phase, in which two $S = 1$ spins at $j = 2i - 1$-th and $2i$-th sites ($\delta > 0$) make a singlet. In this phase, the string order parameters $\mathcal{O}^{z,x}_{\text{string}}$ are zero, so that the hidden discrete symmetry is not broken. We have obtained the phase diagram with the same topology of the quantum Ashkin-Teller model which has the $Z_2 \times Z_2$ symmetry explicitly[10)].

But our phase diagram is not consistent with the previous one by Singh and Gelfand[15)]. They treated the model(1.2) by the series expansion and showed that there exists a multicritical point of the XY, the Haldane, the dimer, and the Néel phases. However, based on the $Z_2 \times Z_2$ symmetry , or the phase diagram of the quantum Ashkin-Teller model, there should be a 2D Gaussian critical line (Haldane-dimer critical line), which contradicts

the phase diagram obtained by Singh and Gelfand.

In our previous paper we mainly studied the BKT transitions (XY-Haldane, XY-dimer). In this paper, we investigate the universality class and the critical properties of not only the XY-Haldane and the XY-dimer transitions but also of the Gaussian transition between the Haldane and the dimer phases, and the 2D Ising transitions of the Néel and the dimer phases. We clarify the relation between the hidden $Z_2 \times Z_2$ symmetry and Haldane-dimer transition, using twisted boundary conditions. We determine the phase boundary and evaluate the critical exponents using the exact diagonalization for the finite size systems.

The organization of this paper is as follows. In the next section, we review the quantum Ashkin-Teller model which has the $Z_2 \times Z_2$ symmetry explicitly, and as its effective theory we consider the sine-Gordon model which describes the information for the critical properties of the model(1.2). In section 3, we study the critical properties of the XY-Haldane and the XY-dimer (BKT type), the Haldane-dimer (2D Gaussian type), and the Haldane-Néel and the dimer-Néel (2D Ising type) transitions using the conformal field theory with the numerical analysis. The last section is the conclusion.

§2. Universality class, $Z_2 \times Z_2$ symmetry and $U(1)$ symmetry

In order to understand the possible phase diagram with the $Z_2 \times Z_2$ symmetry, we review the one dimensional quantum Ashkin-Teller model[16)]

$$H_{AT} = -\sum_j [\sigma_j^z \sigma_{j+1}^z + \tau_j^z \tau_{j+1}^z + \lambda \sigma_j^z \sigma_{j+1}^z \tau_j^z \tau_{j+1}^z] -\beta \sum_j [\sigma_j^x + \tau_j^x + \lambda \sigma_j^x \tau_j^x], \qquad (2.1)$$

where $\sigma_j^{z,x}, \tau_j^{z,x}$ are Pauli matrices. This Hamiltonian is invariant under $\sigma^z \leftrightarrow -\sigma^z$ and $\tau^z \leftrightarrow -\tau^z$ transformations respectively ($Z_2 \times Z_2$ symmetry). For this model(2.1), there is a duality transformation[16)]

$$\tilde{\sigma}_{j+1/2}^x = \sigma_j^z \sigma_{j+1}^z, \quad \tilde{\sigma}_{j+1/2}^z = \prod_{i<j} \sigma_i^x, \qquad (2.2)$$
$$\tilde{\tau}_{j+1/2}^x = \tau_j^z \tau_{j+1}^z, \quad \tilde{\tau}_{j+1/2}^z = \prod_{i<j} \tau_i^x.$$

Under this transformation, the Hamiltonian is transformed as

$$H_{AT}(\lambda, \beta) = \beta H_{AT}(\lambda, 1/\beta),$$

so at $\beta = 1$ the system has the self-duality. It is known that there is the 2D Gaussian critical line ($\beta = 1$, $-1/\sqrt{2} < \lambda < 1$) of continuously varying critical exponents, and at one end ($\beta = 1$, $\lambda = 1$), this line breaks up into two 2D Ising critical lines. At another end of the Gaussian critical line ($\beta = 1$, $\lambda = -1/\sqrt{2}$), it meets two BKT critical lines[17)], so there is a massless region or the "critical fan" in the quantum Ashkin-Teller model. The Gaussian critical line separates the fully ordered and the fully disordered phases about the $Z_2 \times Z_2$ symmetry, and the two 2D Ising critical lines are the boundaries of the partially broken phase.

According to Kohmoto, den Nijs, and Kadanoff[16)], the quantum Ashkin-Teller model(2.1) can be mapped to the $S = 1/2$ XXZ chain with bond-alternation (1.2) ($\Delta = \lambda$, $\delta = (1-\beta)/(1+\beta)$). For this model the Gaussian critical line corresponds to the $\delta = 0$ line ($-1/\sqrt{2} < \Delta < 1$), and at the $\Delta = 1, \delta = 0$ point the bifurcation to the 2D Ising critical lines occurs. The universality class of the $\Delta = 1, \delta = 0$ point is of the level-1 $SU(2)$ Wess-Zumino-Witten(WZW) type[41)].

The effective Hamiltonian of the 1D XXZ model with bond-alternation[20)] (or the quantum Ashkin-Teller model[21)]) is given by

$$H = \frac{1}{2\pi} \int dx \left[vK(\pi\Pi)^2 + \frac{v}{K} \left(\frac{\partial \phi}{\partial x} \right)^2 \right] + \frac{y_1 v}{2\pi a^2} \int dx \cos \sqrt{2}\phi + \frac{y_2 v}{2\pi a^2} \int dx \cos \sqrt{8}\phi, \qquad (2.3)$$

where Π is the momentum density conjugate to ϕ, $[\phi(x), \Pi(x')] = i\delta(x - x')$, a is the lattice constant and v is the sound velocity. The dual field $\theta(x)$ is defined as $\partial_x \theta(x) = \pi \Pi(x)$. Here we make the identification $\phi \equiv \phi + \sqrt{2}\pi, \theta \equiv \theta + \sqrt{2}\pi$, which means the $U(1)$ symmetry for the θ field. For the free field theory ($y_1 = y_2 = 0$), the scaling dimensions of the operators $\exp(\pm im\sqrt{2}\phi)$ and $\exp(\pm in\sqrt{2}\theta)$ are $Km^2/2$ and $n^2/2K$ respectively (where integer variables m and n are magnetic and electric charges in the Coulomb gas picture[22)]). Since the second term of eq.(2.3) is the mass term for the Haldane gap systems, we have $y_1 = 0$ for the half odd integer S XXZ model, and $y_1 \neq 0$ for the integer S XXZ model[20)].

The correspondence between the double sine-Gordon model(2.3) and the quantum Ashkin-Teller model is as follows[16)]

$$y_1 \propto \frac{1-\beta}{1+\beta}, \qquad K = \frac{\pi}{\arccos(\lambda)}.$$

Note that the sine-Gordon model(2.3) is invariant under the transformation

$$\phi \to \phi + \frac{\pi}{\sqrt{2}}, \qquad \theta \to \theta, \qquad y_1 \to -y_1, \qquad \text{and } y_2 \to y_2, \qquad (2.4)$$

which corresponds to the dual transformation(2.2) of the quantum Ashkin-Teller model.

After the scaling transformation $a \to e^{dl}a$, we have the following renormalization group equations.

$$\begin{aligned} \frac{d}{dl}\frac{1}{K} &= \frac{1}{8}y_1^2 + \frac{1}{2}y_2^2, \\ \frac{dy_1}{dl} &= (2 - \frac{K}{2})y_1 - \frac{1}{2}y_1 y_2, \\ \frac{dy_2}{dl} &= (2 - 2K)y_2 - \frac{1}{4}y_1^2. \end{aligned} \qquad (2.5)$$

(This form of equations is previously obtained by Kadanoff[21)].) In Appendix, we show the derivation of these equations. Up to the first order of y's, we see that y_1 is an irrelevant field for $K > 4$ and relevant for $K < 4$, while y_2 is irrelevant for $K > 1$. Thus in the region $K > 1$, we can neglect the third term in eq.(2.3). In this

case, equations (2.5) become

$$\frac{d}{dl}\frac{1}{K} = \frac{1}{8}y_1^2,$$
$$\frac{dy_1}{dl} = (2-\frac{K}{2})y_1,$$

which are the recursion relations of Kosterlitz[18]. There is a separatrix $32K^{-1}-8\ln K^{-1}-y_1^2 = 8+8\ln 4$ $(K>4)$ which separates the infrared unstable region from the infrared stable region, and on this separatrix, BKT transition occurs. On this transition point, logarithmic dependence of finite size spectrum appears, and this makes it difficult to extrapolate to the infinite limit in the numerical calculation.

The line $y_1 = 0$ $(1 < K < 4)$ is the 2D Gaussian critical line, which separates two region. For $1 < K < 4$ and $y_1 \neq 0$, y_1 flows to infinity. For $y_1 > 0$, $\langle\phi\rangle$ renormalized to $\pi/\sqrt{2}$ as $y_1 \to +\infty$ and for $y_1 < 0$, $\langle\phi\rangle \to 0$ as $y_1 \to -\infty$.

The equations (2.5) are invariant under the transformation $y_1 \to -y_1$, but not invariant under $y_2 \to -y_2$. For the $S=1/2$ bond-alternating XXZ chain(1.2), $y_2 > 0$ and at the $SU(2)$ symmetric point ($\Delta = 1$, $\delta = 0$) the Gaussian line separates to two 2D Ising critical lines. There is another possibility other than the Ashkin-Teller multicritical structure, depending on the signature of y_2. When y_2 is negative, the Gaussian line connects to a first order line (*e.g.* $S=1/2$ XXZ chain with staggered field).

In order to identify the excitations with those of the double sine-Gordon model(2.3), we use the following symmetries. The Hamiltonian(1.2) with the periodic boundary condition is invariant under spin rotation around the z-axis, translation by two-sites ($\boldsymbol{S}_i \to \boldsymbol{S}_{i+2}$), space inversion ($\boldsymbol{S}_i \to \boldsymbol{S}_{N-i+1}$) and spin reversal ($S_i^z \to -S_i^z$, $S_j^{\pm} \to -S_j^{\mp}$). Corresponding eigenvalues are $S_T^z \equiv \sum_{i=1}^N S_i^z$, $q = 4\pi n/N$ $(n = 0, \cdots N/2-1)$, $P = \pm 1$ and $T = \pm 1$ respectively. The corresponding symmetry operations in the double sine-Gordon model(2.3) are as follows. The operation to the space inversion (P) is

$$\phi \to -\phi, \quad \theta \to \theta + \pi/\sqrt{2}, \quad x \to -x, \tag{2.6}$$

and the operation to the spin reversal (T) is

$$\phi \to -\phi, \quad \theta \to -\theta + \pi/\sqrt{2}. \tag{2.7}$$

The correspondence of these symmetry operations is summarized in Table 1.

Assuming conformal invariance, the scaling dimension x_n is related to the energy gap of the finite size system with periodic boundary conditions[23]

$$x_n = \frac{L}{2\pi v}\left(E_n(L) - E_g(L)\right), \tag{2.8}$$

where L is the system size, $E_g(L)$ is the ground state energy, and v is the velocity of the system. And the leading finite size correction of the ground state energy is[24, 25]

$$E_g(L) = \epsilon_g L - \frac{\pi v c}{6L}, \tag{2.9}$$

where c is the conformal anomaly number.

In the following section, we calculate these values from small size data of the exact diagonalization with the Lanczos method.

§3. Phase transitions and Numerical results

In this section, we determine the critical points and the universality class. From the hidden $Z_2 \times Z_2$ symmetry and the phase structure of the quantum Ashkin-Teller model, we expect that the XY-Haldane and the XY-dimer transitions are of the BKT type, the Haldane-dimer transition is of the Gaussian type, and the Haldane-Néel and the dimer-Néel transitions belong to the 2D Ising universality class. With the operator structure of the sine-Gordon model(2.3) and the renormalization group analysis, we determined the transition points numerically. To check the universality class, we calculate numerically the conformal anomaly number c and several relations between scaling dimensions.

3.1 Berezinskii-Kosterlitz-Thouless (XY-Haldane and XY-dimer) transitions

First we consider the XY-dimer and the XY-Haldane phase transitions.

For $\delta = 0$ case (XY-Haldane), several numerical studies have been done. For the transition point, Botet and Julian[11] estimated $\Delta_c \sim 0.1$, Sakai and Takahashi [12] $\Delta_c = -0.01 \pm 0.03$, and Yajima and Takahashi[13] $\Delta_c = 0.069 \pm 0.003$. They expected that the transition point is exactly $\Delta = 0$ (see also[26, 27, 28]). In our previous paper, we found that the transition point between the Haldane and the XY phases is exactly $\Delta = 0$ in the numerical accuracy[10].

The effective Hamiltonian for this transition is described by the sine-Gordon model,

$$H = \frac{1}{2\pi}\int dx \left[vK(\pi\Pi)^2 + \frac{v}{K}\left(\frac{\partial\phi}{\partial x}\right)^2\right] + \frac{y_1 v}{2\pi a^2}\int dx \cos\sqrt{2}\phi. \tag{3.1}$$

Here we neglect the third term of eq.(2.3) which is irrelevant for the BKT transition. For this model, there is a special operator, that is the marginal operator

$$\mathcal{M} = -a^2 K(\pi\Pi)^2 + a^2\frac{1}{K}\left(\frac{\partial\phi}{\partial x}\right)^2, \tag{3.2}$$

(this is the Lagrangian density itself for the free field theory) which changes the scaling dimension of scaling operators continuously. For the free field theory, the scaling dimension of $\sqrt{2}\cos\sqrt{2}\phi$ in the second term of eq.(3.1) is $K/2$, and the BKT transition occurs when this dimension becomes 2, *i.e.*, the renormalized K is 4.

Besides the operators $\mathcal{M}$ and $\sqrt{2}\cos\sqrt{2}\phi$, $\sqrt{2}\sin\sqrt{2}\phi$ and $\exp(\mp i4\sqrt{2}\theta)$ are also marginal at the BKT transition point. Recently Nomura[29] studied the structure of these operators near the transition point. He found that the $\sqrt{2}\cos\sqrt{2}\phi$ and the marginal operator $\mathcal{M}$ are hybridized in the course of the renormalization, to satisfy the orthogonality condition of scaling operators. We set the scaling dimensions of $\sqrt{2}\cos\sqrt{2}\phi$-like, $\sqrt{2}\sin\sqrt{2}\phi$, $\exp(\mp i4\sqrt{2}\theta)$ and marginal-like operators as x_1, x_2, x_3 and x_0. We denote K and y_1 as $K = 4 + 2y_0$ and

$y_1 = \pm y_0(1+t)$ near the BKT critical point ($y_1 = \pm y_0$). Since the scaling dimension is related to the excitation energy as eq.(2.8), Nomura found the finite size behaviors of scaling dimensions up to the first order of y_0 and y_1 as

$$\begin{aligned} x_1(l) &\equiv \frac{L\Delta E_1(L)}{2\pi v} = 2 + 2y_0(l)(1+\frac{2}{3}t), \\ x_2(l) &\equiv \frac{L\Delta E_2(L)}{2\pi v} = 2 + y_0(l), \\ x_3(l) &\equiv \frac{L\Delta E_3(L)}{2\pi v} = 2 - y_0(l), \\ x_0(l) &\equiv \frac{L\Delta E_0(L)}{2\pi v} = 2 - y_0(l)(1+\frac{4}{3}t), \end{aligned} \tag{3.3}$$

where we define $l = \log L$. From the recursion relations of Kosterlitz(2.6) for $t = 0$, we have $y_0(l) = 1/\log(L/L_0)$ (L_0 is a constant), so logarithmic corrections appear. At the transition point the scaling dimensions x_0 and x_3 cross linearly, and this means that at the critical point there exists a degeneracy of excited states. So we can determine the BKT transition point by the level crossing of these excitations, and we can also eliminate the logarithmic corrections by the appropriate average of the excitations. From table.1, the first $S_T^z = 0, q = 0, P = T = 1$ [x_0] and the $S_T^z = \pm 4, q = 0, P = 1$ [x_3] excitations degenerate on the BKT line. Note that in the $S_T^z = \pm 1, P = -1$ subspace the lowest excitations correspond to the operators $\exp(\mp i\sqrt{2}\theta)$ whose scaling dimension is $x_4 = 1/8$ ($\eta = 1/4$) at the BKT transition point.

In numerical calculations, we study finite rings of N sites ($N = 8, 10, 12, 14, 16$) with periodic boundary conditions. We determine the velocity v by the current field ($x = 1$, $q = 2\pi/L$),

$$v = \lim_{L\to\infty} \frac{\Delta E(L, k = 2\pi/L)}{2\pi/L},$$

where L is the system size and $L = N/2$ in the considering case. To obtain this value, we extrapolated the value of the finite size system as $v(L) = v + \text{const}/L^2$. The leading finite size corrections of eq.(2.8) come from the operators $L_{-2}\bar{L}_{-2}\mathbf{1}$ and $((L_{-2})^2 + (\bar{L}_{-2})^2)\mathbf{1}$[23, 30, 31] which are the descendant fields of the identity operator. The scaling dimensions of these operators are 4, and the leading correction term of the scaling dimension(2.8) behaves as $1/L^2$. (Here we neglect the corrections from third term of eq.(2.3) because the scaling dimension of $\sqrt{2}\cos\sqrt{8}$ is $2K$, bigger than 4.) In Fig.2(a) we show the excitation energies for $N = 16, \Delta = -0.5$. We determine the XY-dimer phase boundary by the crossing point of excitations $S_T^z = 0, P = T = 1$ and $S_T^z = \pm 4, P = 1$. Figure 2(b) shows the excitation energies for $N = 16$, $\Delta = 0$. In this case one of the states ($S_T^z = 0$, $q = 0$, $P = T = 1$) and the eigenstate ($S_T^z = \pm 4$, $q = 0$, $P = 1$) are exactly degenerate on the whole line, thus in our previous paper we have concluded that the XY-Haldane phase boundary is on exactly $\Delta = 0$. We determine the multi-critical point of the XY, the dimer, and the Haldane phases by the crossing point of excitations $S_T^z = \pm 4$, $P = 1[x_3]$ and $S_T^z = 0$, $P = T = -1[x_2]$ on the $\Delta = 0$ line. This point corresponds to $K = 4$ and $y_1 = 0$ in the continuum Hamiltonian (3.1). Figure 3 shows the size dependence of this multi-critical point, and we have estimated the multi-critical point as $\Delta = 0, \delta = 0.230 \pm 0.001$.

In our previous paper, we have presented the size dependence of $(x_0 + x_2)/2$ and $(2x_0 + x_1)/3$ to verify that the transition is of the BKT type. From eqs.(3.3), these values eliminate the logarithmic corrections and we have seen that these converge to 2 as the system size increases. In Fig.4 we show the extrapolated values along the BKT critical line. From eqs.(3.3), the average $(3x_0 + x_1 + x_2)/5$ also eliminates the logarithmic corrections, where the coefficient 3, 1, 1 is the degeneracy at the critical point. Figure 5 shows the size dependence of it, where $1/N^2$ behavior comes from corrections of the irrelevant operators $L_{-2}\bar{L}_{-2}\mathbf{1}$ and $((L_{-2})^2 + (\bar{L}_{-2})^2)\mathbf{1}$. In Fig.6 we show the extrapolated values along the BKT critical line. We have estimated the conformal anomaly number using eq.(2.9), as $c = 0.998$ for $\Delta = -0.5$, $\delta = 0.583$ and $c = 1.000$ for $\Delta = 0$, $\delta = 0$, also considering the finite size correction of the $x = 4$ irrelevant field. Hence we conclude that the transitions are of the BKT-type.

Next, we show the asymptotic behavior near the BKT critical point. From eqs.(3.3), we can remove the t linear terms as

$$\frac{1}{3}[x_0(l) + x_1(l) + x_3(l)] = 2 + \mathcal{O}(y_0^2). \tag{3.4}$$

In Fig.7, we show this value near the critical points $\Delta = -0.5$, $\delta = 0.583$ and $\Delta = 0$, $\delta = 0$. The linear components of t are almost absent.

Lastly, we consider the XY region where the energy gap is zero and the spin correlations decay in the power law. The scaling dimensions of the operators $\exp(\mp i\sqrt{2}\theta)$ [x_4] and $\exp(\mp i2\sqrt{2}\theta)$ [x_5] are $x_4 = 1/2K$ and $x_5 = 2/K$, so the ratio of these values is $x_5/x_4 = 4$. These operators correspond to the lowest states ($S_T^z = \pm 1$, $q = 0$, $P = -1$) and ($S_T^z = \pm 2$, $q = 0$, $P = 1$) respectively. On the BKT transition point, we have

$$\begin{aligned} x_4(l) &= \frac{1}{8} - \frac{y_0}{16}, \\ x_5(l) &= \frac{1}{2} - \frac{y_0}{4}, \end{aligned} \tag{3.5}$$

so this ratio is correct up to the first order of the logarithmic correction $y_0(l) = 1/\log(L/L_0)$. Figure 8 shows the extrapolated values of this ratio for $\Delta = -0.5$. The evaluated values are almost 4, except near the BKT transition point. The discrepancy near the transition point comes from the higher order logarithmic corrections [$\mathcal{O}(1/(\ln L)^2)$].

In the XY region, the product $x_2 \cdot x_3$ is 4 up to $\mathcal{O}(1/(\ln L)^2)$ (from eqs.(3.3)) near the transition point, since the field x_2 is free from the effect of the hybridization. (Contrary to this, the product $x_1 \cdot x_3$ is affected from the bybridization of x_0 and x_1, so there remains $calO(1/\ln L)$ correction.) In Fig.9, this product value is presented and we can see the expected value.

In Fig.10, we show the scaling dimension x_0 of the marginal operator $\mathcal{M}$ of the $N = 16$ system. On the transition point the deviation from 2 is more than 10 %.

The deviation of x_0 from 2 comes from the hybridization with the operator $\sqrt{2}\cos\sqrt{2}\phi$. Near the transition point we can eliminate this effect of the hybridization taking the combination $x_0 + x_1 - x_2 = 2$, and so this value eliminate the logarithmic correction up to the first order of y_0. In Fig.10 we show the extrapolated value of $x_0(l) + x_1(l) - x_2(l)$, and the discrepancy decreases in a few percent.

3.2 Gaussian (Haldane-dimer) transition

Next, let us consider the Haldane-dimer transition. In the dimer phase, the system has no symmetry breaking, whereas in the Haldane phase, the system exhibits the hidden $Z_2 \times Z_2$ symmetry breaking. For this transition, the operator $\sqrt{2}\cos\sqrt{2}\phi$ in eq.(2.3) is relevant($4 > K > 1$) and the Gaussian transition occurs at $y_1 = 0$.

3.2.1 Determination of the transition point

In the content of the VBS picture, for even site systems with periodic boundary conditions, the Haldane gap state of $S = 1$ systems can be written as[34)]

$$(a_N^\dagger b_1^\dagger - b_N^\dagger a_1^\dagger)\prod_{j=1}^{N-1}(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)|0\rangle, \tag{3.6}$$

and the dimer state can be

$$\prod_{k=1}^{N/2}(a_{2k-1}^\dagger b_{2k}^\dagger - b_{2k-1}^\dagger a_{2k}^\dagger)^2|0\rangle \quad (\delta > 0), \tag{3.7}$$

or

$$(a_N^\dagger b_1^\dagger - b_N^\dagger a_1^\dagger)^2 \prod_{k=1}^{N/2-1}(a_{2k}^\dagger b_{2k+1}^\dagger - b_{2k}^\dagger a_{2k+1}^\dagger)^2|0\rangle \quad (\delta < 0),$$

where we describe the spin state by the Schwinger bosons, that is, $a_j^\dagger$ ($b_j^\dagger$) creates the $S = 1/2 \uparrow (\downarrow)$ spin at the j-th site. These two states have the same symmetries which conserve the Hamiltonian, especially the space inversion $j \to N - 1 + j$ ($P = 1$) and the spin reversal $a^\dagger \leftrightarrow b^\dagger$ ($T = 1$). For the periodic boundary conditions, the ground state is singlet in both the Haldane and the dimer phases. So we cannot expect the simple finite size scaling behaviors near the critical points.

But the situation is different for another boundary condition, *i.e.*, the twisted boundary condition $S_{N+1}^x = -S_1^x$, $S_{N+1}^y = -S_1^y$, $S_{N+1}^z = S_1^z$. For this boundary condition, the Haldane gap state is written as

$$(a_N^\dagger b_1^\dagger + b_N^\dagger a_1^\dagger)\prod_{j=1}^{N-1}(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)|0\rangle, \tag{3.8}$$

while the dimer state can be

$$\prod_{k=1}^{N/2}(a_{2k-1}^\dagger b_{2k}^\dagger - b_{2k-1}^\dagger a_{2k}^\dagger)^2|0\rangle \quad (\delta > 0), \tag{3.9}$$

or

$$(a_N^\dagger b_1^\dagger + b_N^\dagger a_1^\dagger)^2 \prod_{k=1}^{N/2-1}(a_{2k}^\dagger b_{2k+1}^\dagger - b_{2k}^\dagger a_{2k+1}^\dagger)^2|0\rangle \quad (\delta < 0).$$

The Haldane state has $P = -1$, $T = -1$, but the dimer state has $P = 1$, $T = 1$, so these two states have the different P and T eigenvalues, and the energy eigenvalues cross at the critical point.

For the sine-Gordon model, we can explain this as follows. First, let us consider the following 1-D Hamiltonian with periodic boundary condition

$$H = H_0 + \frac{\lambda}{2\pi}\int_0^L dx\mathcal{O}_1, \tag{3.10}$$

where H_0 is the fixed point Hamiltonian, L is the system length (setting the ultraviolet cutoff as 1), and $\mathcal{O}_1$ is a scaling operator whose scaling dimension is x_1 ($\mathcal{O}_1^\dagger = \mathcal{O}_1$). According to Cardy[23)], the following size dependence of excitation energy up to the first order perturbation is obtained

$$\Delta E_n = \frac{2\pi v}{L}\left(x_n + \lambda C_{n1n}\left(\frac{2\pi}{L}\right)^{x_1-2} + \cdots\right), \tag{3.11}$$

where x_n is the scaling dimension of the operator $\mathcal{O}_n$, and C_{n1n} is the operator product expansion (OPE) coefficient of the operators $\mathcal{O}_n$ and $\mathcal{O}_1$. We assume that the operator $\mathcal{O}_1$ is a relevant one ($x_1 < 2$). Up to the first order perturbation theory, we find that at the critical point $\lambda = 0$ the scaled gap $L\Delta E_n$ does not depend on the system size besides finite size corrections of irrelevant operators. But if the OPE coefficient C_{n1n} is zero, the first order perturbation theory is not sufficient and we must consider the second order term of λ in eq.(3.11). In such a case the scaled gap $L\Delta E_n$ has some extremum at the critical point.

In the sine-Gordon model, the relevant operator is $\mathcal{O}_1 = \sqrt{2}\cos\sqrt{2}\phi$, and there is no operator $\mathcal{O}_n$ which has nonzero value of C_{n1n}. It is related with the charge neutrality conditions in the Coulomb gas picture[22)]. (Note that the operators $e^{\pm i\phi/\sqrt{2}}$ is not allowed by the identification $\phi \equiv \phi + \sqrt{2}\pi$.) Thus the OPE coefficient in eq.(3.11) is zero, and we cannot use the usual finite size scaling method. In other words, the Haldane gap systems with the periodic boundary condition does not have the local "order parameter" which has non-zero value of OPE coefficient with the relevant operator in the Hamiltonian[8)].

Second, let us see what happens for the twisted boundary condition $S_{N+1}^x \pm iS_{N+1}^y = e^{\pm i\Phi}(S_1^x \pm iS_1^y)$, $S_{N+1}^z = S_1^z$. It has been known that for the primary operator $\exp(i\sqrt{2}m\phi + i\sqrt{2}n\theta)$, the effect of the boundary condition $\Phi = \pi$ is to shift the magnetic charge m by one half[19)] $m \to m - 1/2$, $n \to n$. If the half magnetic charges exist, we have the following size dependence of the scaling dimensions of the half magnetic charge operators $\sqrt{2}\cos\phi/\sqrt{2}$ [x_6] and $\sqrt{2}\sin\phi/\sqrt{2}$ [x_7] as[32)]

$$\begin{aligned} x_6(L) &= \frac{L(E_6(L, \Phi = \pi) - E_g(L, \Phi = 0))}{2\pi v} \\ &= \frac{K}{8} + \frac{y_1}{2}\left(\frac{2\pi}{L}\right)^{K/2-2} + \cdots, \\ x_7(L) &= \frac{L(E_7(L, \Phi = \pi) - E_g(L, \Phi = 0))}{2\pi v} \\ &= \frac{K}{8} - \frac{y_1}{2}\left(\frac{2\pi}{L}\right)^{K/2-2} + \cdots. \end{aligned} \tag{3.12}$$

We see that these two energy eigenvalues cross linearly

at $y_1 = 0$.

Note that the sine-Gordon model(2.3) is invariant under the transformation(2.4). The half magnetic charge operator $\sqrt{2}\cos\phi/\sqrt{2}$ ($\sqrt{2}\sin\phi/\sqrt{2}$) corresponds to the operator $P = \sigma^z\tau^z$ ($\tilde{P} = \tilde{\sigma}^z\tilde{\tau}^z$)[33] of the quantum Ashkin-Teller model. Under this transformation, the half magnetic charge operators $\sqrt{2}\cos\phi/\sqrt{2}$ and $\sqrt{2}\sin\phi/\sqrt{2}$ are transformed as

$$\sqrt{2}\cos\frac{1}{\sqrt{2}}\phi \to -\sqrt{2}\sin\frac{1}{\sqrt{2}}\phi,$$
$$\sqrt{2}\sin\frac{1}{\sqrt{2}}\phi \to \sqrt{2}\cos\frac{1}{\sqrt{2}}\phi. \qquad (3.13)$$

Thus at the point $y_1 = 0$, the system has the self-duality in the quantum Ashkin-Teller language. By the invariance of eq.(2.4), the third term of eq(2.3) does not affect the determination of the crossing point for eq.(3.12).

Numerically, with $\Phi = \pi$ boundary condition we determine the phase boundary of the Haldane and dimer phases for $N = 8, 10, 12, 14, 16$ systems. In Fig.11, we show two low lying energies of the subspace $\sum S^z = 0$ with the boundary condition $S^x_{N+1} = -S^x_1$, $S^y_{N+1} = -S^y_1$, $S^z_{N+1} = S^z_1$ for $\Delta = 0$, 0.5 and 1, which correspond to $E_6(L,\Phi=\pi) - E_g(L,\Phi=0)$ and $E_7(L,\Phi=\pi) - E_g(L,\Phi=0)$. From figures of $\Delta = 0.5$, 1.0, we see that in the Haldane phase $P = T = -1$ state is lower than $P = T = 1$ state but in the dimer phase the relation reverses as expected.

However, contrary to the $S = 1/2$ case, since the self-duality at $y_1 = 0$ is not exact for $S = 1$ bond-alternating system, the crossing point of E_6 and E_7 has a size dependence as $\mathcal{O}(N^{-2})$ (or $\mathcal{O}(N^{-4})$) (see appendix B). Figure 3($\Delta = 0$) and Figure 12($\Delta = 0.5$) show the size dependence of the crossing points. In fact, assuming the size dependence of the crossing point $\delta_c(N) = \delta_c(\infty) + aN^{-b}$, we can check the power b, using the relation

$$\frac{\ln\left(\frac{\delta_c(N+2)-\delta_c(N)}{\delta_c(N)-\delta_c(N-2)}\right)}{\ln\left(\frac{N+1}{N-1}\right)} = -b - 1 + \mathcal{O}\left(\frac{1}{N^2}\right). \qquad (3.14)$$

Figure.13 shows the exponet evaluated with this method. Hereafter we extrapolate the critical point as $\delta_c(N) = \delta_c(\infty) + aN^{-2} + bN^{-4}$.

3.2.2 *Check of the universality class*

In Fig.14, we show the value K estimated from x_1,x_2, x_4, and x_6 of the $N = 16$ system. These values are almost consistent except near $\Delta = 1$ where the effect of the logarithmic corrections of the level-1 $SU(2)$ WZW model[41] appears.

We estimated the conformal anomaly number at the critical point $\Delta = 0.5$, $\delta = 0.2524$ as $c = 0.998$. In Table 2, we show some extrapolated scaling dimensions for $\Delta = 0.5$. The estimation of K is consistent in each others.

For the Gaussian transitions the leading finite size corrections of eq.(2.8) come from the operators $L_{-2}\bar{L}_{-2}\mathbf{1}$ and $((L_{-2})^2 + (\bar{L}_{-2})^2)\mathbf{1}$ or $\sqrt{2}\cos\sqrt{8}\phi$, of which the third operator is included in the third term of eq.(2.3). The scaling dimensions of these operators are 4 and $2K$ ($1 < K < 4$) respectively. By the third term of eq.(2.3), at $y_1 = 0$ only the scaling dimensions x_1 and x_2 are corrected as

$$x_1(L) = \frac{K}{2} + \frac{y_2}{2}\left(\frac{1}{L}\right)^{2K-2} + \cdots,$$
$$x_2(L) = \frac{K}{2} - \frac{y_2}{2}\left(\frac{1}{L}\right)^{2K-2} + \cdots.$$

We can eliminate this correction by summing these two dimensions. To improve the precision of the 1-parameter scaling, hereafter we try to eliminate the effect of the y_1, y_2 fields, at least first order.

We show the extrapolated values of x_0 on the Haldane-dimer transition lines in Fig.15. The discrepancy is about 30 % at $\Delta = 1$. Figure 16 shows the extrapolated values of

$$x_4 \cdot (x_6 + x_7) = \frac{1}{2K} \cdot \left(\frac{K}{8} + \frac{K}{8}\right),$$

and the obtained values are consistent with 1/8 except near $\Delta = 1$, where the discrepancy (about 15 %) comes from the logarithmic corrections of higher orders. In Fig.17, we present the ratio x_4 and x_5. Figure 18 shows the extrapolated values of $(x_1 + x_2) \cdot x_4$ which should be 4. The summation of x_1 and x_2 eliminate the correction from the third term of eq.(2.3). In Fig.19, we present the ratio $(x_1+x_2)/(x_6+x_7)$ where the numerator is the value with the periodic boundary condition and the denominator is with the $\Phi = \pi$ twisted boundary condition.

Last of this subsection, we remark that the method to determine the transition point can also apply to determine the Gaussian fixed point ($y_1 = 0$) in the XY phase. In Fig.1, we also show the Gaussian fixed line. We find that the line ends at the point $\Delta = -1$, $\delta = 0$. Near this point, the Gaussian line behaves as $\delta \propto (1 + \Delta)^{1/4}$ (see Fig.20).

3.3 *Isotropic case*

The isotropic case $\Delta = 1$ has been studied in relation with the Affleck-Haldane prediction. Affleck and Haldane[35,36] considered the $\Delta = 1$ case for the arbitrary S case, mapping onto the nonlinear $O(3)$ σ-model. They showed that the topological angle θ is given by $\theta = 2\pi S(1-\delta)$ and the system should be massless when $\theta/2\pi$ is half odd integer. Numerically several authors estimated the transition point δ_c. For $S = 1$ case, they concluded $\delta_c \simeq 0.25 \pm 0.01$ and $c = 1$[37,38,39]. Totsuka *et. al.*[39] extensively studied this case, and obtained the critical dimensions up to the logarithmic corrections and identified the universality class as the $SU(2)$ level-1 Wess-Zumino-Witten model.

For $y_1 = 0$, the RG equations are given by

$$\frac{d}{dl}\frac{1}{K} = \frac{1}{2}y_2^2,$$
$$\frac{dy_2}{dl} = 2(1-K)y_2. \qquad (3.15)$$

Denoting $K = 1 + y_0/2$ near $K = 1$, we have

$$\frac{dy_0}{dl} = -y_2^2,$$

$$\frac{dy_2}{dl} = -y_0 y_2.$$

The WZW point is $y_0 = y_2$. According to Giamarchi and Schulz[40], and Nomura[29], we obtain the following scaling dimensions

$$\begin{aligned}
x_0(l) &= 2 - y_0(l)\left(1 + \frac{4}{3}t\right), \\
x_1(l) &= \frac{1}{2} + \frac{3}{4}y_0(l)\left(1 + \frac{2}{3}t\right), \\
x_2(l) &= \frac{1}{2} - \frac{1}{4}y_0(l)(1 + 2t), \\
x_4(l) &= \frac{1}{2} - \frac{1}{4}y_0(l), \\
x_5(l) &= 2 - y_0(l), \\
x_8(l) &= 2 + 2y_0(l)\left(1 + \frac{2}{3}t\right), \\
x_9(l) &= 2 + y_0(l),
\end{aligned} \tag{3.16}$$

where t is defined as $y_2 = y_0(1+t)$, and we define the scaling dimensions of $\sqrt{2}\cos\sqrt{8}\phi$ and $\sqrt{2}\sin\sqrt{8}\phi$ as x_8 and x_9 respectively. At $t = 0$ we have $y_0(l) = 1/\log(L/L_0)$ and the eqs.(3.16) are consistent with the non-Abelian bosonization theory[41].

From these equations, we see that $(x_1(l) + 3x_4(l))/4$, $(x_0(l) + x_9(l))/2$, $(2x_0(l) + x_8(l))/3$, and $(5x_0 + 3x_9 + x_8)/9$ do not depend on the logarithmic corrections at the Wess-Zumino-Witten point.

We obtained the transition point with the same method in the previous subsection. The obtained value is $\delta_c = 0.2598$. The conformal anomaly number is estimated as $c = 0.990$. The extrapolated value of $(x_1(l)+3x_4(l))/4$ is 0.495. and the extrapolated values of $(x_0(l)+x_9(l))/2$, $(2x_0(l)+x_8(l))/3$, and $(5x_0+3x_9+x_8)/9$ are 1.982, 2.026, and 1.997 respectively.

3.4 2D Ising (Haldane-Néel and dimer-Néel) transition

Lastly, we study the Néel-Haldane and the Néel-dimer transitions. Because in the Néel phase, the hidden $Z_2 \times Z_2$ symmetry is partly breaking, we see that the broken symmetry of these transitions is the Z_2 symmetry.

On the Néel-Haldane transition ($\Delta = 1.17 \pm 0.02$, $\delta = 0$), Nomura[14] calculated the critical exponents as $\nu = 0.98 \pm 0.007$, $\beta = 0.126 \pm 0.007$,$\eta = 0.253 \pm 0.002$, with a (large cluster decomposition) Monte Carlo method. Later Sakai and Takahashi[12] reexamined this transition using the phenomenological renormalization group method and finite-size scaling technique, and obtained $\nu = 1.02 \pm 0.05$, $\gamma/\nu = 1.76 \pm 0.01$, and $\eta = 0.23 \pm 0.01$. These results are consistent with the 2D Ising universality class ($\nu = 1$, $\beta = 1/8$, $\eta = 1/4$, $\gamma = 7/4$). So here we consider the Néel-dimer transition and check its universality class.

In $c < 1$ conformal field theory, the current field does not exist, so we cannot determine the velocity by the same method as the $c = 1$ case.

Assuming the 2D Ising transition, we expect that the first excitation state has the $S^z_T = 0$, $q = 0$, $P = T = -1$ symmetry, and this corresponds to the order parameter σ of the Ising model, whose scaling dimension is $1/8$. The scaling dimension of the level-1 descendant field $\hat{L}_{-1}\sigma$ is $1 + 1/8$, so we can determine the velocity of the system by

$$v = \frac{E_{\hat{L}^{-1}\sigma} - E_\sigma}{2\pi L}. \tag{3.17}$$

Using this velocity we can determine the conformal anomaly number c and scaling dimensions of several excitations.

Numerically we determined the phase boundary by the phenomenological renormalization group method, that is, evaluating the crossing point of the scaled gaps $N\Delta E(N)$ and $(N+2)\Delta E(N+2)$ for $N = 6, 8, 10, 12, 14$ systems with periodic boundary conditions. Using the velocity(3.17), we estimate the conformal anomaly number as $c = 0.4997$ and the scaling dimensions as $x_\sigma = 0.126$ and $x_\epsilon = 1.001$, for $\Delta = 2.0$, $\delta = 0.683$. In figure 21, we show low lying scaling dimensions of the dimer-Néel transition point, where circle shows $S^z_T = 0$, $P = T = 1$, and cross shows $S^z_T = 0$, $P = T = -1$ states. These values are consistent with the prediction from the Ising universality.

§4. Conclusion

We discussed the critical properties of the $S = 1$ bond-alternating XXZ spin chains. The expected phases are the ferromagnetic, the XY, the Haldane gap, the dimer, the Néel phases. First, we considered the universality class based on the hidden $Z_2 \times Z_2$ symmetry. Then we have taken the analogy from the quantum Ashkin-Teller model which has a $Z_2 \times Z_2$ symmetry explicitly. The effective model of the quantum Ashkin-Teller model is the double sine-Gordon model, and using the information of it, we determined the XY-Haldane, the XY-dimer and the Haldane-dimer phase boundaries numerically. For the XY-Haldane and the XY-dimer (BKT) transition, the renormalization group aspect is important and it is difficult to apply the simple finite size scaling method due to the logarithmic corrections. While for the Gaussian transition between the Haldane and the dimer phases, we adapted the twisted boundary condition to obtain the preferable operator structure and determined the transition point by a level crossing. This method can also be applied to determine the Gaussian fixed line in the XY phase. We found that the hidden discrete symmetry is crucial for the phase transition and the topology of the phase diagram. We also identified the universality class numerically using the conformal field theory and eliminating the correction of the (marginal) irrelevant fields.

It is interesting to consider the arbitrary spin case. Oshikawa[44] studied the arbitrary S Heisenberg chain with bond-alternation in the VBS picture. It was pointed out that the successive dimerization transition occurs in the Affleck-Haldane prediction[45]. Oshikawa calculated the string order parameter, and concluded that for the successive dimerization, the breakdown of the hidden $Z_2 \times Z_2$ symmetry occurs. Considering the phase diagram of the quantum Ashkin-Teller and the Haldane's conjecture, we predicted in our previous paper that for arbitrary S XXZ spin chains with bond-alternation, there

are $2S+1$ BKT lines, $2S$ 2D Gaussian lines, and $2S+1$ 2D Ising lines in the region $-1 < \delta < 1$(summarized in table 3). For $S = 3/2$ isotropic case $\Delta = 1$, Yajima and Takahashi[46] studied with the density matrix renormalization group method evaluate the transition point as $\delta = 0, \pm 0.42$.

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Appendix A: Renormalization group equations

We derive the renormalization group equations(2.5). Let us consider the following Euclidean action,

$$\mathcal{S} = \mathcal{S}_0 + \sum_\alpha \frac{\lambda_\alpha}{2\pi} \int \frac{d^2\boldsymbol{r}}{a^2} \mathcal{O}_\alpha(z,\bar{z}), \tag{A·1}$$

where $\mathcal{S}_0$ is a fixed point action, a is a ultraviolet cutoff, $\boldsymbol{r} = (v\tau, x)$, and $z = v\tau + ix$, $\bar{z} = v\tau - ix$,. . We set the scaling operator $\mathcal{O}_\alpha$ as the normalized one as

$$\langle \mathcal{O}_\alpha(z_1,\bar{z}_1)\mathcal{O}_\beta(z_2,\bar{z}_2)\rangle_0 = \frac{\delta_{\alpha,\beta}}{\left(\frac{z_1-z_2}{a}\right)^{2h_\alpha}\left(\frac{\bar{z}_1-\bar{z}_2}{a}\right)^{2\bar{h}_\alpha}}, \tag{A·2}$$

where $z_1 = v\tau + ix$, $\bar{z}_1 = v\tau_1 - ix_1$ and h and $\bar{h}$ are the conformal weights and the scaling dimension of $\mathcal{O}_\alpha$ is $x_\alpha = h_\alpha + \bar{h}_\alpha$.

According to Zamolodchikov[47], and Ludwig and Cardy[48], we have the following one loop renormalization group equations for the scaling transformation $a \to a' = e^{dl}a$

$$\frac{d\lambda_\alpha}{dl} = (2 - x_\alpha)\lambda_\alpha - \sum_{\beta,\gamma} \delta_{h^\alpha_{\beta\gamma},\bar{h}^\alpha_{\beta\gamma}} \frac{C_{\alpha\beta\gamma}}{2}\lambda_\beta\lambda_\gamma, \tag{A·3}$$

where $h^\alpha_{\beta\gamma} = h_\alpha - h_\beta - h_\gamma$, and $C_{\alpha\beta\gamma}$ is the operator product expansion coefficient of $\mathcal{O}_\alpha$, $\mathcal{O}_\beta$, and $\mathcal{O}_\gamma$.

For the double sine-Gordon model(2.3), we define

$$\mathcal{S}_0 = \frac{1}{2\pi K}\int d^2\boldsymbol{r} \left[\left(\frac{\partial\phi}{v\partial\tau}\right)^2 + \left(\frac{\partial\phi}{\partial x}\right)^2\right],$$

$$\mathcal{O}_0 = \frac{a}{K}\left[\left(\frac{\partial\phi}{v\partial\tau}\right)^2 + \left(\frac{\partial\phi}{\partial x}\right)^2\right],$$

$$\mathcal{O}_1 = \sqrt{2}\cos\sqrt{2}\phi,$$

$$\mathcal{O}_2 = \sqrt{2}\cos\sqrt{8}\phi,$$

where $\mathcal{O}_0$ is proportional to the Lagrangian density. Using

$$\langle\phi(z,\bar{z})\phi(0,0)\rangle_0 = -\frac{K}{2}\log\frac{|z|}{a},$$

and Wick's theorem, we can easily derive the following operator product expansions

$$\mathcal{O}_1(z,\bar{z})\mathcal{O}_0(0,0) = -\frac{K}{2}\frac{1}{|z/a|^2}\mathcal{O}_1(0,0) + \cdots, \tag{A·4}$$

$$\mathcal{O}_2(z,\bar{z})\mathcal{O}_0(0,0) = -2K\frac{1}{|z/a|^2}\mathcal{O}_2(0,0) + \cdots, \tag{A·5}$$

$$\begin{aligned}\mathcal{O}_1(z,\bar{z})\mathcal{O}_1(0,0) = &-\frac{K}{2}\frac{1}{|z/a|^{K/2-2}}\mathcal{O}_0(0,0) \\ &+\frac{1}{\sqrt{2}}\frac{1}{|z/a|^{-K}}\mathcal{O}_2(0,0) + \cdots,\end{aligned} \tag{A·6}$$

where '$\cdots$' dose not include $\mathcal{O}_0$, $\mathcal{O}_1$, and $\mathcal{O}_2$. From these equations we have

$$C_{011} = C_{101} = C_{110} = -\frac{K}{2},$$

$$C_{022} = C_{202} = C_{220} = -2K,$$

$$C_{112} = C_{121} = C_{211} = \frac{1}{\sqrt{2}}.$$

Using these OPEs and eq.(A·3), we can derive the renormalization group equations(2.5).

Appendix B: Correction of the Gaussian fixed line

Our method in §3.2 to determine the Gaussian fixed line is affected by the descendant fields (critical dimension $x = K/2 + 2n$; n:integer) of the $\sqrt{2}\cos\sqrt{2}\phi$ field, since generally the self-duality (in the Ashkin-Teller language) is not exact for the finite size system. Considering correction terms from the descendant fields of $\sqrt{2}\cos\sqrt{2}\phi$ and $L_2\bar{L}_2\mathbf{1}$, $((L_2)^2 + (\bar{L}_2)^2)\mathbf{1}$ $(x = 4)$ irrelevant fields, we obtain

$$x_{6,7}(L) \tag{B·1}$$

$$= \frac{K}{8} \pm \frac{y_1}{2}\left(\frac{2\pi}{L}\right)^{K/2-2} \pm \sum_{n=1}^{\infty}\frac{c_n}{2}\left(\frac{2\pi}{L}\right)^{K/2+2n-2} + dL^{-2},$$

since the OPE coefficient

$$\langle\sqrt{2}\cos\phi/\sqrt{2}|\sqrt{2}\cos\sqrt{2}\phi|\sqrt{2}\cos\phi/\sqrt{2}\rangle$$

changes sign under the transformation(2.4). Therefore, the crossing points behave

$$y_1^{\mathrm{cross}}(L) = -\sum_1^{\infty} c_n\left(\frac{2\pi}{L}\right)^{-2n}. \tag{B·2}$$

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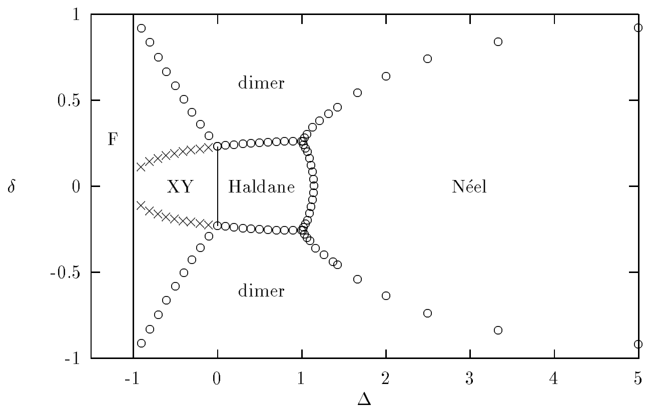

Fig. 1. Phase diagram in the $\Delta-\delta$ plane. The XY-dimer and the XY-Haldane phase boundaries are of the BKT type, the dimer-Haldane boundary is of the 2D Gaussian type, and the Néel phase boundaries are of the 2D Ising type. We also show the Gaussian fixed line ($y_1 = 0$) in the XY region ($\times$).

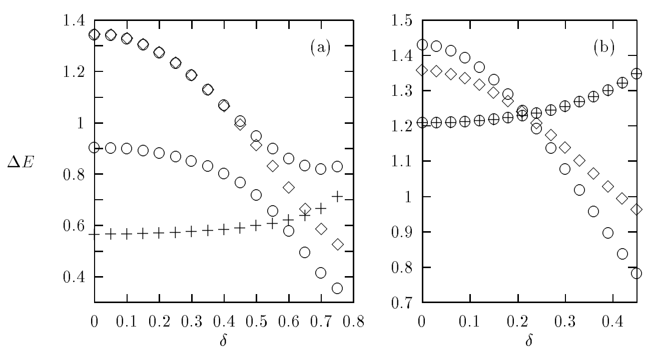

Figure 1:

Fig. 2. Excitation energies for (a) $N = 16$, $\Delta = -0.5$ and (b) $N = 16$, $\Delta = 0$. $\bigcirc$'s are $S^z_T = 0$, $q = 0$, $P = T = 1$ excitations, $\diamond$ is S^z_T, $q = 0$, $P = T = -1$ excitations, and $+$ is the $S^z_T = \pm 4$, $q = 0$, $P = 1$ excitation.

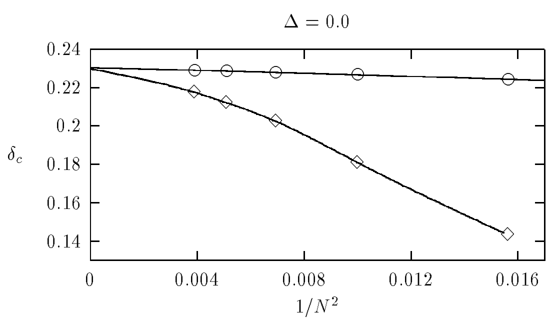

Fig. 3. The size dependence of the BKT multicritical point. $\diamond$: the crossing point of ($S^z_T = 0$, $k = 0$, $P = T = -1$) and ($S^z_T = \pm 4$, $k = 0$, $P = 1$) excitations; Circles are obtained by the system with the twisted boundary condition(§3.2).

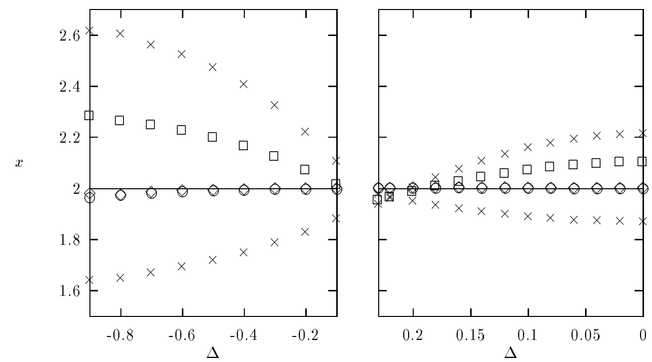

Fig. 4. The extrapolated values of $(2x_0 + x_1)/3(\diamond)$ and $(x_0 + x_2)/2(\bigcirc)$ along the BKT transition lines. We also show the bare values of $x_0(\times)$, $x_1(\times)$, and $x_2(\square)$ of the $N = 16$ system.

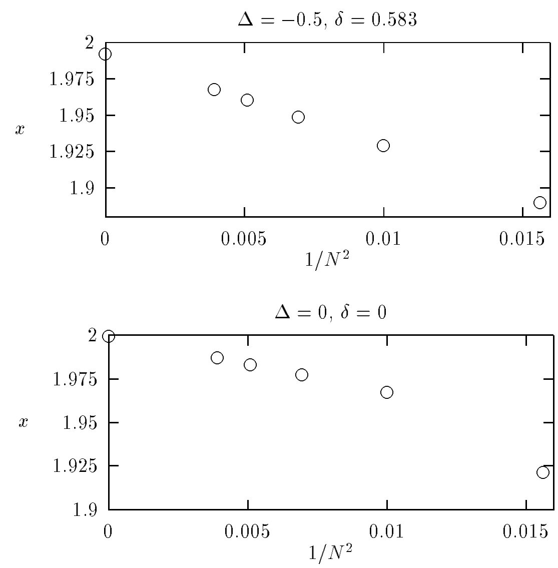

Fig. 5. The size dependence of $(3x_0 + x_1 + x_2)/5$ as a function of $1/N^2$.This behavior comes from the $x = 4$ irrelevant operators.

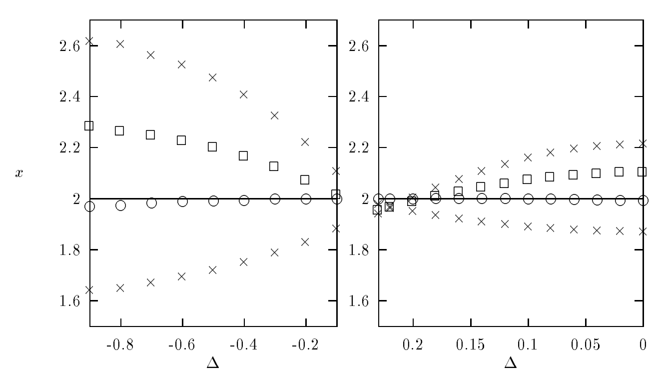

Fig. 6. The extrapolated values of $(3x_0 + x_1 + x_2)/5$ ($\bigcirc$) along the BKT transition lines.

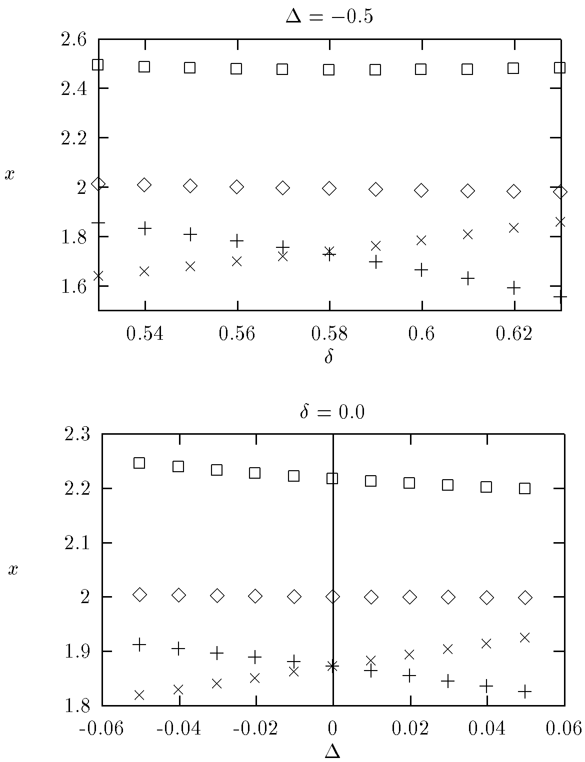

Fig. 7. The extrapolated values of $(x_0 + x_1 + x_3)/3$ near the BKT critical point($\diamond$). We also show the bare values of $x_0(\times)$, $x_1(\square)$, and $x_3(+)$ of the $N = 16$ system.

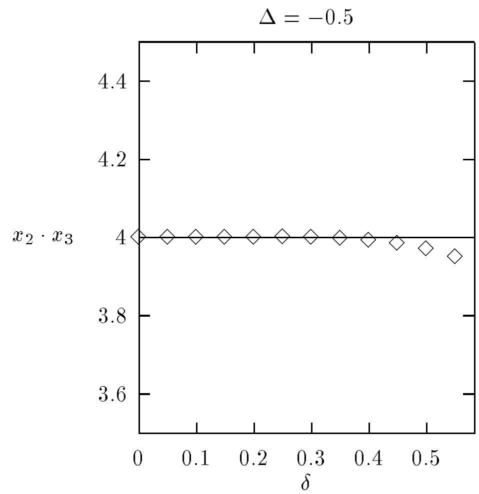

Fig. 9. The extrapolated values of $x_2 \cdot x_3$ in the XY phase.

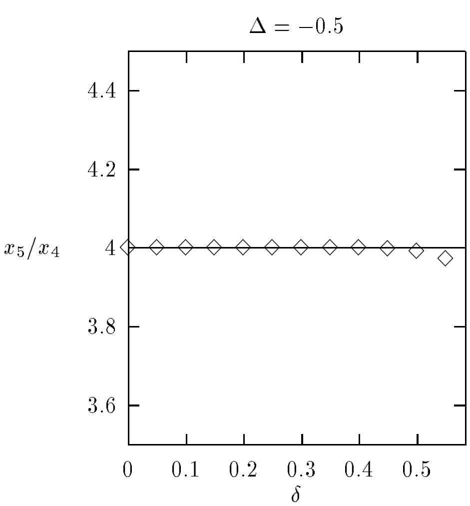

Fig. 8. The extrapolated values of x_5/x_4 in the XY phase. The transition point is $\Delta = -0.5$, $\delta = 0.583$.

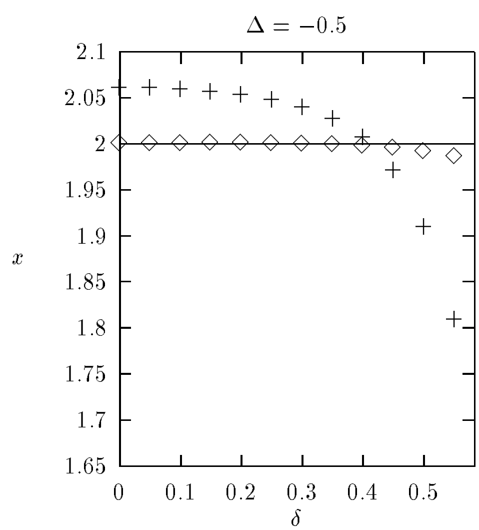

Fig. 10. $+$: The scaling dimension of the marginal operator of the $\Delta = -0.5$,$N = 16$ system. $\diamond$: The extrapolated values of $x_0 + x_1 - x_2$ which eliminates the logarithmic corrections.

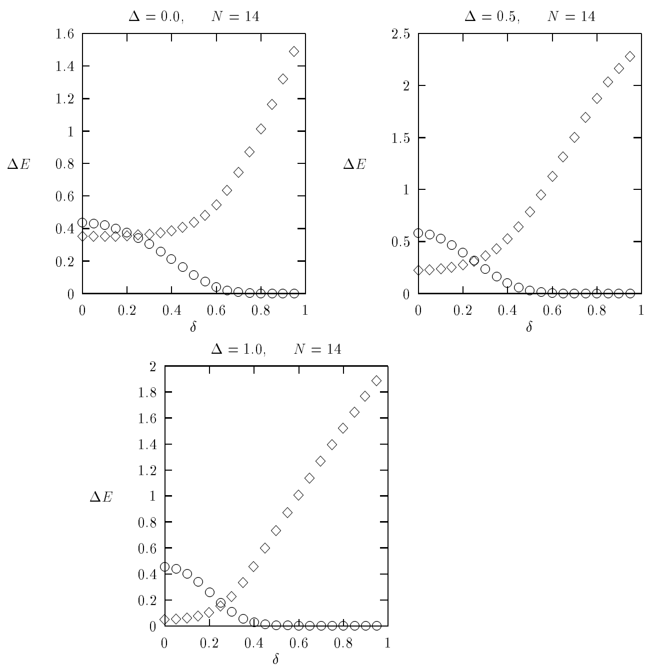

Fig. 11. Energy difference $E_6(\pi) - E_g(0)$ (◯) and $E_7(\pi) - E_g(0)$(◇). ◇ is the state with $\sum S^z = 0$, $P = T = -1$, and ◯ is the state with $\sum S^z = 0$, $P = T = 1$.

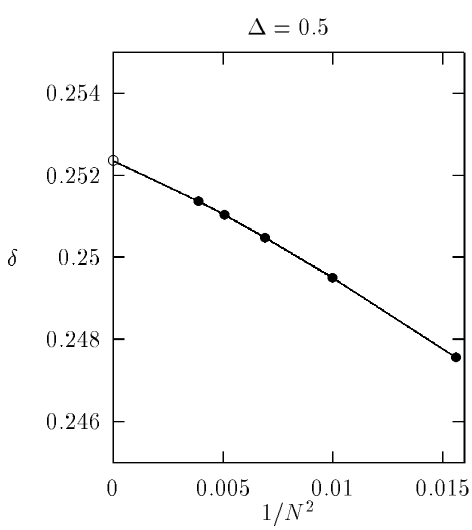

Fig. 12. Size dependence of the crossing points. The extrapolated value is $\delta_c = 0.2524$.

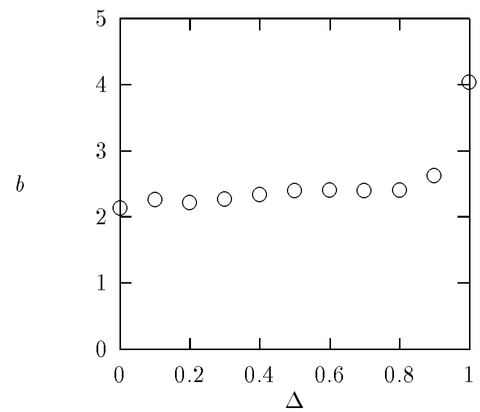

Fig. 13. The evaluated value of the exponent b form eq.(25) for $N = 14$.

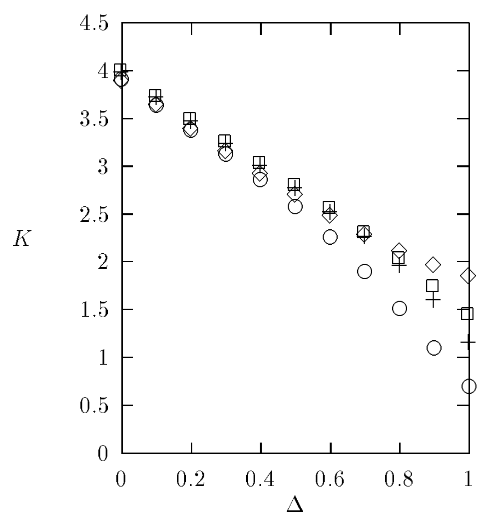

Fig. 14. The obtained values of K for $N = 16$ systems from x_1(◇), x_2(◯), x_4(□), and x_6(+).

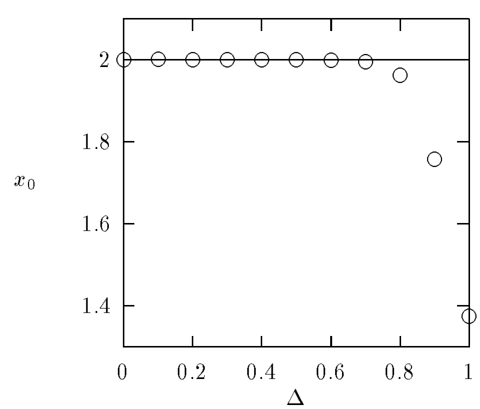

Fig. 15. The extrapolated values of x_0 which is the scaling dimension of the marginal operator.

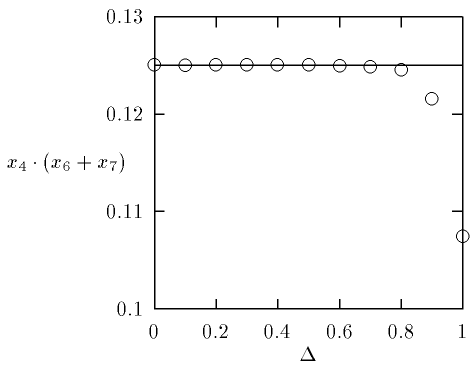

Fig. 16. The extrapolated values of $x_4 \cdot (x_6 + x_7)$ on the Haldane-dimer critical line.

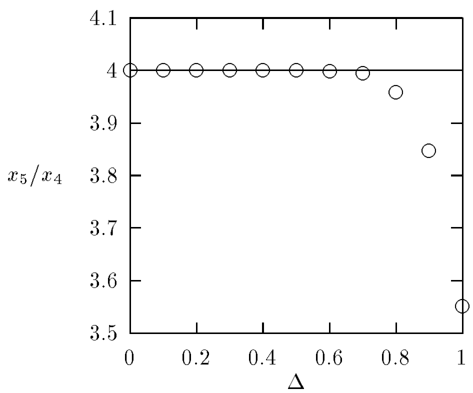

Fig. 17. The extrapolated ratio between x_5 and x_4.

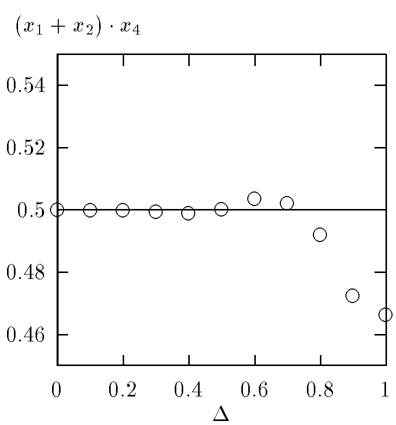

Fig. 18. The extrapolated values of $(x_1 + x_2) \cdot x_4$.

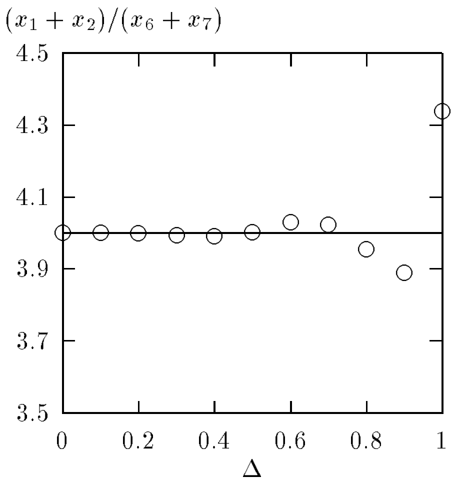

Fig. 19. The extrapolated values of $(x_1+x_2)/(x_6+x_7)$.

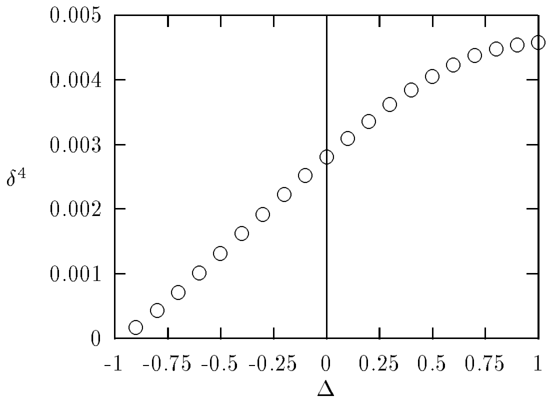

Fig. 20. The Gaussian fixed line in the $\delta^4-\Delta$ plane. K takes a value from ∞ to 1 in the region $\Delta:[-1,1]$. Near $\Delta=-1$, the Gaussian fixed line behaves as $\delta \propto (1+\Delta)^{1/4}$.

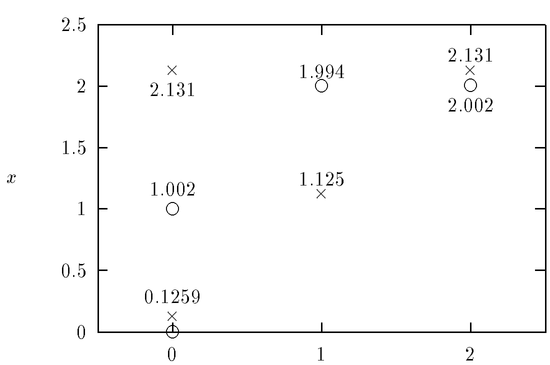

Fig. 21. The low lying scaling dimensions of the dimer-Néel transition point $\Delta=2.0$, $\delta=0.683$. Horizontal line is the momentum $\times L/2\pi$. $\bigcirc$ is the scaling dimensions of $P=T=1$ states, and $\times$ is of $P=T=-1$ states.

Symmetry operation				Operators of	Notation of
q	S^z_T	P	T	sine-Gordon model	scaling dimensions
0	0	1	1	$\mathcal{M}$	x_0
0	0	1	1	$\sqrt{2}\cos\sqrt{2}\phi$	x_1
0	0	-1	-1	$\sqrt{2}\sin\sqrt{2}\phi$	x_2
0	± 4	1		$\exp \mp i4\sqrt{2}\theta$	x_3
0	± 1	-1		$\exp \mp i\sqrt{2}\theta$	x_4
0	± 2	1		$\exp \mp i2\sqrt{2}\theta$	x_5
	0	1	1	$\sqrt{2}\cos\phi/\sqrt{2}$*	x_6
	0	-1	-1	$\sqrt{2}\sin\phi/\sqrt{2}$*	x_7
0	0	1	1	$\sqrt{2}\cos 2\sqrt{2}\phi$	x_8
0	0	-1	-1	$\sqrt{2}\sin 2\sqrt{2}\phi$	x_9

Table 1: Correspondence of symmetry operations. *:These two operators are defined with the $\Phi = \pi$ twisted boundary condition.

scaling dimension	$x_{1,0} = 1/2K$	$x_{0,1} = K/2$	$x_{0,1/2} = K/8$
	0.179	1.41	0.350

Table 2: Scaling dimensions at the critical point $\Delta = 0.5$, $\delta = 0.252$. Here we extrapolated the corrections from the irrelevant field $L_2\bar{L}_2\mathbf{1}$ ($x = 4$).

S	2-D Gaussian line	BKT line	2-D Ising line
$1/2$	1	2	2
1	2	3	3
S	$2S$	$2S+1$	$2S+1$

Table 3: The number of transition lines for arbitrary spins.